

3-(4-Chlorophenyl)-3-trimethylsilyloxy-acrylonitrile (isomer 2)

Other names: 3-(4-Chlorophenyl)-2-propenenitrile-3-ol trimethylsilyl ether (isomer 2)
InChI: InChI=1S/C12H14ClNOSi/c1-16(2,3)15-12(8-9-14)10-4-6-11(13)7-5-10/h4-8H,1-3H3/b12
InchiKey: JVWMJYOBGOEWEK-XYOKQWHBSA-N
Formula: C12H14ClNOSi
SMILES: C[Si](C)(C)OC(=CC#N)c1ccc(Cl)cc1
Mol. weight [g/mol]: 251.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Crippen Method
logp	4.056		Crippen Method
rinpol	1731.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U378235&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/37-674-3/3-4-Chlorophenyl-3-trimethylsilyloxy-acrylonitrile-isomer-2.pdf>

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